

# Transport properties of doped $t$ - $J$ ladders

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Conductivity and Hall coefficient for various types of  $t$ - $J$  ladders are calculated as a function of temperature and frequency by numerical diagonalization. A crossover from an incoherent to a coherent charge dynamics is found at a temperature  $T_{\text{coh}}$ . There exists another crossover at  $T_{\text{PG}}$  below which a pseudogap opens in the optical spectra, induced by the opening of a spin gap. In the absence of the spin gap,  $T_{\text{coh}}$  and the coherent weight are suppressed especially with increasing dimensionality. On the contrary,  $T_{\text{coh}}$  is strongly enhanced by the pseudogap formation below  $T_{\text{PG}}$ , where the coherent Drude weight decreases with increasing dimensionality. The Hall coefficient shows a strong crossover at  $T_{\text{PG}}$  below which it has large amplitude for small doping concentration.

In high- $T_c$  cuprates, transport phenomena in the normal state show various unusual properties in terms of standard normal metals. It is well known that the in-plane DC conductivity,  $\sigma$ , is proportional to  $1/T$  with  $T$  being the temperature<sup>1</sup>, and the AC conductivity has a broad incoherent part well fitted by  $\sigma(\omega) \propto 1/\omega^2$ . Another peculiarity exists in the Hall coefficient,  $R_H$ . At low  $T$ 's, in spite of the electron density less than half filling,  $R_H$  is usually positive, meaning hole-like carriers, with a large amplitude scaled as  $1/\delta$  with hole doping  $\delta$ <sup>3,4</sup>. It also shows a crossover to a small amplitude at a rather high temperature,  $T_{\text{cr}}$ , and  $T_{\text{cr}}$  rapidly decreases with increasing  $\delta$ <sup>5,6</sup>. These behaviors are incompatible with the standard Fermi liquid theory, implying that the carriers change their character with  $T$  due to strong correlations. The incoherent charge dynamics and strongly  $T$ -dependent Hall coefficient have been analyzed in terms of criticality near the Mott transition together with the effects of preformed pairs<sup>7</sup>. Jaklič and Prelovšek<sup>8</sup> calculated  $\sigma(\omega, T)$  for the two-dimensional (2D)  $t$ - $J$  model using Lanczos diagonalization. Their results reproduced the above features of the high- $T_c$  cuprates, in contrast to the 1D  $t$ - $J$  model, which is known to have a very coherent  $\sigma(\omega)$ <sup>9</sup>.

Assaad and Imada showed a large crossover in the  $T$ -dependence of the high-frequency Hall coefficient,  $R_H^*$ , for the 2D Hubbard model using quantum Monte Carlo simulations<sup>10</sup>. At small  $\delta$ 's,  $R_H^*$  changes its sign twice with decreasing  $T$  from  $T=\infty$ : from negative to positive at  $T_U$ , and then back to negative at  $T_{\text{AF}}$ . In the region of  $T_{\text{AF}} < T < T_U$ , it is found that strong correlations substantially suppress a quantum coherence between different spin configurations in the electron motion, leading to a large positive Hall coefficient expected for a spinless Fermion case. Within numerical results, the 2D Hubbard model shows no definite indications for preformed pairing or superconductivity. It neither reproduces the experimentally observed  $T$ -dependence of  $R_H$ .

Recently several two-leg ladder compounds have been experimentally studied. A finite spin gap was con-

firmed in the insulating phases, and the superconductivity was reported for doped  $\text{Sr}_{14-x}\text{Ca}_x\text{Cu}_{24}\text{O}_{41}$  under high pressure<sup>11</sup>. The optical conductivity in the metallic region shows a similar incoherent character to the high- $T_c$ 's while the resistivity follows  $\rho \propto T^2$  at low  $T$ 's in the normal phase<sup>12</sup>.

In this paper, we study the conductivity and Hall coefficient of the  $t$ - $J$  two-leg ladders. The Hamiltonian of the  $t$ - $J$  ladder under a magnetic field,  $B$ , perpendicular to the ladder plane is written as

$$\mathcal{H} = \sum_{\langle i,j \rangle} \left[ \sum_{\sigma} \left( -t_{ij} c_{j\sigma}^{\dagger} c_{i\sigma} + \text{H.c.} \right) + J_{\alpha} \mathbf{S}_i \cdot \mathbf{S}_j \right], \quad (1)$$

where the site sum is taken over nearest neighbor pairs, and the label,  $\alpha=x(y)$ , denotes the leg (rung) direction. The exchange constant is  $J_x = J$  along legs and  $J_y = J'$  along rungs. The hopping integral has a finite phase due to the magnetic field,  $t_{ij} = t \exp[-ie \int_{\mathbf{r}_i}^{\mathbf{r}_j} \mathbf{A}(\mathbf{r}) \cdot d\mathbf{r}]$ , with the Landau gauge,  $\mathbf{A} = B(-y, 0, 0)$ . The periodic (open) boundary conditions are used along the leg (rung) direction.

The conductivity at temperature  $T$  is defined by the Kubo formula as

$$\sigma_{\alpha\beta}(\omega) = \frac{ie^2}{V} \frac{1}{\omega + i\eta} \left( -\langle K_{\alpha} \rangle \delta_{\alpha\beta} - \frac{1}{Z} \sum_{n,m} \frac{e^{-E_m/T} - e^{-E_n/T}}{E_n - E_m - \omega - i\eta} \langle n | J_{\alpha} | m \rangle \langle m | J_{\beta} | n \rangle \right), \quad (2)$$

where  $V$  is the number of sites,  $Z = \text{Tr} e^{-\mathcal{H}/T}$ ,  $|n\rangle$ 's are eigenstates of  $\mathcal{H}$  with energies  $E_n$ ,  $\langle K_{\alpha} \rangle$  is the thermal average of the kinetic energy along the  $\alpha$ -direction, and  $J_{\alpha}$  is the paramagnetic current operator.  $\eta$  is an adiabatic constant. The Hall coefficient is defined as

$$R_H(\omega) = \frac{1}{B} \frac{\sigma_{xy}(\omega)}{\sigma_{xx}(\omega)\sigma_{yy}(\omega) + \sigma_{xy}^2(\omega)}. \quad (3)$$

Shastry et al. suggested its high-frequency limit as a measure of  $T$ -dependent effective carrier density<sup>13</sup>

$$R_H^* \equiv \lim_{\omega \rightarrow \infty} R_H(\omega) = \frac{V}{iB} \frac{\langle [J_x, J_y] \rangle}{\langle -K_x \rangle \langle -K_y \rangle}. \quad (4)$$

We have numerically obtained all the eigenstates using the Householder method, and calculated the conductivity and the Hall coefficient using Eqs. (2)-(4). The canonical ensemble is used to fix the electron number with all the subspaces of  $S_{\text{tot}}^z$  included. Spin gap,  $\Delta_s$ , is also calculated as the difference of the ground state energy between the subspaces of  $S_{\text{tot}}^z = 0$  and 1.

Let us start with the  $\omega$ -dependence of conductivity. Figure 1 shows  $\sigma_{xx}(\omega)$  at various  $T$ 's for three typical cases: (a) uniformly coupled ladder (UL),  $J/t=J'/t=0.3$ , (b) rung-dominant ladder (RL) which has larger rung couplings than leg couplings,  $J'/t=20J/t=6.0$ , and (c) dimerized ladder (DL) where each chain is dimerized,  $J/t=J'/t=0.3$ , and  $J''/t=1.0$ . To characterize the dimerization, we use the notation  $J=J_{2j}<J''=J_{2j+1}$ . At high  $T$ 's above the temperature scale of  $\Delta_s$ ,  $\sigma_{xx}(\omega)$  has a broad incoherent part. At these temperatures, the conductivity is well fitted by the scaling function proposed by Jaklič and Prelovšek for the 2D  $t$ - $J$  model<sup>14</sup>

$$\sigma_{xx}(\omega) = \frac{1 - e^{-\omega/T}}{\omega} C(\omega). \quad (5)$$

Here  $C(\omega)$  is a smooth universal function with a broad width,  $\gamma_0$  of the order of several times of  $t$ . In our case, this may be well approximated by  $C(\omega) \sim C_0(T)e^{-(\omega/\gamma_0)^2} [1 - e^{-(\gamma_0/T + T/\omega)}]$  for small  $\eta$  with a rather weak  $T$  dependence of  $C_0(T)$ . The details will be discussed elsewhere. The broad structure of  $C(\omega)$  is a consequence of rapid and incoherent charge dynamics, since as shown from Eq. (2),  $C(\omega)$  is the current-current correlation function,  $C(\omega) = \int dt \langle J(t)J(0) \rangle e^{i\omega t}$ . We note that this incoherent charge dynamics is consistent with the anomalous suppression of coherence near the Mott insulator derived in the scaling theory<sup>7</sup>. It should also be noted that this scaling function with weak  $T, \omega$  dependence of  $C(\omega)$  corresponds to the relaxation rate proposed in the marginal Fermi liquid theory<sup>15</sup>  $\tau^{-1} \sim \max(\omega, T)$  at low  $\omega$  and  $T$ .

Below a characteristic temperature,  $T_{\text{PG}}$ , the conductivity  $\sigma_{xx}(\omega)$  turns to show a pseudogap at  $\omega \leq \omega_{\text{PG}}$  as clearly shown in Fig. 1 (b) and (c). This is accompanied by the appearance of a prominent coherent peak in the low- $\omega$  region, particularly for Fig. 1 (b), and its weight grows with decreasing  $T$ . By changing  $J$  and  $J'$ , we have found that  $T_{\text{PG}} \simeq \Delta_s \simeq \omega_{\text{PG}}$ . Note that  $\Delta_s = 2.402$  for (b) and  $\Delta_s = 0.812$  for (c). The magnetic susceptibility,  $\chi(T)$ , is in fact substantially reduced at  $T < T_{\text{PG}}$ . In the case of Fig. 1 (a), the pseudogap behavior is not prominent down to the lowest temperature used in the calculation because of the small spin gap  $\Delta_s/t \approx 0.002$ .

Comparing Fig. 1 (b)(namely RL) and (c)(DL) at  $T < T_{\text{PG}}$ , it is noticed that the RL has a larger coherent weight. The observed  $1/\omega^2$ -behavior of  $\sigma_{xx}(\omega)$  at  $\omega/t \lesssim 1$  in (b) is actually due to a finite  $\eta$ . The  $\eta$ -dependence

at small  $\eta$  indicates that this coherent peak is indeed a  $\delta$ -function,  $\pi D^* \delta(\omega)$ , within our numerical results, although  $T > 0$ . In contrast,  $\sigma_{xx}(\omega)$  for the DL in Fig. 1 (c) shows a larger incoherent weight, even below  $T_{\text{PG}}$ .

The pseudogap behavior below  $T_{\text{PG}}$  indicates the formation of singlet bound pairs of electrons, which behave as singlet hard-core bosons. This is consistent with the exact diagonalization results at  $T = 0$ <sup>16-18</sup>. The part of  $\omega < \Delta_s$  and  $T < T_{\text{PG}}$  is therefore described by an effective model of hard-core bosons with charge  $+2e$ , belonging to the universality class of Luther-Emery liquids<sup>19</sup>.

The bound pairs are formed on a rung in the RL's while on a dimerized strong bond in the DL's. Therefore it leads to different effective models, i.e., hard-core bosons on a single *chain* and on a *ladder*, respectively, with a small nearest-neighbor hopping  $t^*$  and interactions  $V^*$  as calculated in Ref.<sup>17</sup>. The boson ladder and chain show an incoherent behavior, above a characteristic temperature,  $T_{\text{coh}}$ , which is similar to the incoherent behavior of the Fermion ladder at  $T \gtrsim T_{\text{PG}}$  discussed for Fig. 1. Whereas a dissipationless Drude peak,  $\sigma_{xx}(\omega) \sim \pi D^*(T) \delta(\omega)$ , appears below  $T_{\text{coh}}$  with  $D^*(T) \approx \text{const.}$   $T_{\text{coh}}$  also corresponds to the crossover in the  $T$ -dependence of the kinetic energy: roughly speaking,  $\langle K_x \rangle \propto 1/T$  above  $T_{\text{coh}}$  and  $\langle K_x \rangle \approx \text{const.}$  below it. Based on a finite-size scaling of  $\langle K_x \rangle(T)$ , we found  $T_{\text{coh}} \propto \delta^2 t^*$ , consistent with the prediction of the scaling theory for the metal-insulator transition in 1D<sup>7</sup>.

The  $\sigma(\omega, T)$  of the boson chain was calculated by Zotos and Prelovšek<sup>20</sup>. They found that there remains a real  $\delta$ -function of the Drude peak even at temperatures of order  $t^*$ , and attributed it to the integrability of the model. Our results are consistent with their observation.

We have calculated the conductivity by the same numerical method for hard-core boson chains and ladders. The results show that the Drude weight for the boson ladders is smaller than for the boson chains, suggesting a more diffusive character of the conductivity, whereas it turns out that  $T_{\text{coh}}$  is higher for the ladders. The scaling theory for a single component system<sup>7</sup> predicted  $D \propto \delta$  and  $T_{\text{coh}} \propto \delta^2$  in 1D, and  $D \propto \delta$  and  $T_{\text{coh}} \propto \delta$  in 2D. The difference between the results in Fig. 1 (b) and (c) implies a crossover from 1D to 2D.

Now let us discuss the Hall coefficient at  $\omega \rightarrow \infty$ ,  $R_H^*$ . Figure 2 shows the  $T$ -dependence of  $R_H^*$  for various ladders including those used for Fig. 1. In the limit of  $T \rightarrow \infty$ ,  $R_H^*$  is finite and positive in all cases. For the  $t$ - $J$  ladder with hole doping  $\delta$ , it is indeed given by  $\lim_{T \rightarrow \infty} R_H^* = -\frac{\delta}{1-\delta} + \frac{1-\delta}{4\delta}$ , identical to the result for the square lattice<sup>13</sup>, where it is positive if  $0 < \delta < \frac{1}{3}$ . With lowering  $T$ ,  $R_H^*$  decreases and becomes negative at a certain temperature,  $T_{\text{AF}}$ , as in the case of the 2D Hubbard model<sup>10</sup>. It suggests the same origin of this behavior with the 2D case at  $T < T_{\text{AF}}$ , i.e., the gradual formation of electron-like large "Fermi surface" in the presence of two spin species.

In the UL's ( $J/t=J'/t=0.3$  and 1.5),  $R_H^*$  remains neg-

ative at  $T < T_{AF}$ . With decreasing  $T$ , it shows a minimum and finally converges to a large negative value at  $T=0$ . In the RL's ( $J/t=0.3$ ,  $J'/t=6.0$  and  $20.0$ ),  $R_H^*$  decreases with lowering  $T$  as in the previous case, but there appears a spike-like structure at around  $T_{PG}$ . This structure is more prominent for larger  $J'$ 's. In the DL's,  $R_H^* < 0$  in a very narrow  $T$ -region and  $R_H^*$  increases to positive and converges to a large positive value at  $T=0$ .

The low-temperature behaviors, particularly at  $T < T_{PG}$ , depend on the coupling constants, meaning distinct characters of charge carriers for the different cases. Since  $\langle -K_\alpha \rangle > 0$  at any  $T$ 's, the sign of  $R_H^*$  is determined by the sign of  $\langle [J_x, J_y] \rangle$ , i.e., that of  $\sigma_{xy}$ . Considering the formation of bound hole pairs below  $T_{PG}$ , it is natural to assume that  $\sigma_{xy}$  in Eq. (3) is obtained as the sum of contributions from bound pairs and unpaired electrons. The  $T$ -dependence of  $R_H^*$  is therefore qualitatively explained from  $T$ -dependence of the density and mobility of these two types of carriers.

As for the unpaired electrons, their density decreases exponentially at  $T < T_{PG}$ . Equation (4) shows their Hall mobility is determined by the processes of moving an unpaired electron first along one direction and then perpendicular to it. It is important to notice that the effective hopping matrix elements of unpaired electrons acquire an extra Fermion negative sign when they undergo a recombination scattering with a bound pair. Therefore, the Hall mobility of unpaired electrons is positive at  $T > T_{AF}$  and  $T \ll T_{PG}$  while negative at  $T_{PG} < T < T_{AF}$ , changing its sign twice.

When the bound pairs are concerned, we recall that  $\sigma_{xy}$  at  $T \ll T_{PG}$  is mainly determined by this part, since only few unpaired electrons are thermally excited. The bound pairs are formed on the rungs in the RL's, whereas within the legs for the DL's. The opposite sign of the Hall mobility at  $T < T_{PG}$  between these two cases may be attributed to these different local configurations of bound pairs, which will be discussed elsewhere.

The Hall coefficient for small  $\omega$  is shown in Fig. 3 for the same ladders in Fig. 2. The  $T$ -dependence is qualitatively similar to  $R_H^*$  for the UL's and the DL's. On the other hand, the RL's have a different  $T$ -dependence at small  $\omega$ 's. This may be due to finite size corrections, since  $R_H$  at small  $\omega$ 's is very sensitive to the value of the adiabatic constant  $\eta$ . Absolute value of  $R_H$  in Fig. 3 (a)-(d) also changes considerably with varying  $\eta$ .

Figure 4 shows the hole doping dependence of  $R_H^*$  at  $T=0$  calculated by Lanczos diagonalization for the UL's. When the electron density is small,  $R_H^* < 0$ , meaning electron-like. When  $\delta \geq \frac{1}{2}$ , the value of  $R_H^*$  is close to the classical value, i.e.,  $R_H^{\text{class}} = -\frac{1}{1-\delta} < R_H^*(T=0) < R_H^*(T=\infty) < 0$ , showing little  $J$ -dependence. The Hall coefficient in this region is mainly determined by the electron density. On the other hand, at small  $\delta$ 's,  $R_H^*$  shows a substantial  $J$ -dependence, and when  $J/t > 1$  it is rather close to  $1/\delta$  except for its negative sign. This means the importance of electron correlation effects and

is consistent with the previous conclusion that the bound pairs are effective charge carriers. A comment is necessary for the positive sign of  $R_H^*$  at  $\delta = \frac{1}{8}$  and  $J/t < 0.2$ . This may be due to strong ferromagnetic fluctuations. As shown in Ref.<sup>17</sup>, the Nagaoka ferromagnetic ground state appears near half filling at small  $J$ 's. The "Fermi volume" of the electrons with the majority spin is doubled, leading to a hole-like  $R_H^*$ .

We finally discuss on how the Hall coefficient is affected when ladders are coupled. Figure 5 shows  $R_H^*(T=0)$  for various *coupled ladders* calculated by Lanczos diagonalization using Eq. (4). Two two-leg ladders are coupled by interladder hopping  $t_L$  and exchange  $J_L$ , to form a  $4 \times 4$ -site cluster. The finite coupling of the ladders shows shifts of  $R_H^*$  toward the positive direction in general. A typical case is weakly coupled DL's and its equivalent configurations (for example,  $J'' > J = J' = 10J_L = 0.3t$  or  $0.03J' > J = J'' = 10J_L = 0.3t$  or  $0.6J' > J = J'' = J_L = 0.3t$ ). A few exceptions with the negative  $R_H^*$  are the cases of (i) weakly coupled RL's, (ii) the configuration of weakly coupled plaquettes (e.g., the coupled DL at  $J_L < J < J'' \leq J'$ ). The crossover from a small to a large positive  $R_H$  at  $T_{PG}$  in 2D configurations is reminiscent of the crossover in the cuprates at  $T = T_{cr}$ , suggesting that it shares the same mechanism due to preformed pairs below  $T_{PG}$ <sup>7</sup>.

In summary, the frequency-dependent conductivity and Hall coefficient of various types of doped ladders were calculated by numerical diagonalization. There is a crossover from high- $T$  incoherent to low- $T$  coherent dynamics with the appearance of the Drude peak. Its crossover temperature  $T_{coh}$  is enhanced by the spin gap and resultant pseudogap formations.  $T_{coh}$  increases with increasing dimensionality when the spin gap is formed, although the coherent weight itself decreases. The Hall coefficient shows a strong crossover to large amplitudes at low temperatures below the spin-gap temperature.

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FIG. 1. Frequency dependence of the conductivity of the  $t$ - $J$  ladder for various choices of parameters. (a)  $J=J'=0.3t$ , 2 holes in  $2\times 6$  sites, (b)  $J=0.3t$ ,  $J'=6.0t$ , 2 holes in  $2\times 6$  sites, and (c)  $J=J'=0.3t$ ,  $J''=t$ , 2 holes in  $2\times 4$  sites. The adiabatic constant is (a)-(b):  $\eta=0.1t$ , (c):  $0.01t$ . (d)  $I(\omega) = \int_0^\omega C(\omega')d\omega'$  calculated for (a).

FIG. 2. Temperature dependence of the high-frequency Hall coefficient of the  $t$ - $J$  ladder. The system size is (a)-(b): 2 holes in  $2\times 6$  sites, and (c) 2 holes in  $2\times 4$  sites.

FIG. 3. Temperature dependence of the low-frequency Hall coefficient of the  $t$ - $J$  ladder. The system size is (a)-(b): 2 holes in  $2\times 6$  sites ( $\delta = \frac{1}{6}$ ), and (c) 2 holes in  $2\times 4$  sites ( $\delta = \frac{1}{4}$ ). The adiabatic constant is  $\eta = 0.1t$ .

FIG. 4. Electron-density dependence of  $R_H^*$  for the  $t$ - $J$  ladder with uniform couplings,  $J=J'$ .  $2\times 8$  sites.

FIG. 5. Hall coefficient of coupled  $t$ - $J$  ladders in the  $\omega=\infty$  limit,  $R_H^*$ . Two ladders with  $4\times 2$  sites are coupled by inter-ladder hopping  $t_L$  and exchange  $J_L$ .











